Ensemble Learning

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IIT Gandhinagar

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Based on Ensemble methods in ML by Dietterich
Three reasons why ensembles make sense:

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1) Statistical: Sometimes if **data is limited, many competing hypotheses can be learned** all giving the same accuracy on training data.

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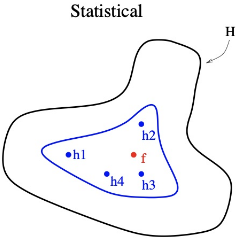
1) Statistical: Sometimes if **data is limited, many competing hypotheses can be learned** all giving the same accuracy on training data.

E.g., we can learn many decision trees for the same data giving the same accuracy.



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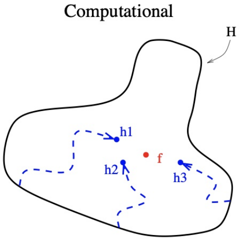
E.g., decision trees employ greedy criteria



3) Representational: Some **classifiers/regressors cannot learn the true form or representation.**

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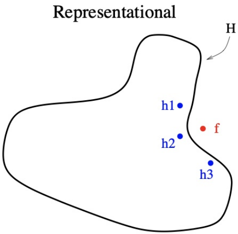
E.g., decision trees can only learn axis-parallel splits.



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1) A necessary and sufficient condition for an ensemble of classifiers to be more accurate than any of its individual members is if the classifiers are accurate and diverse.
2) An accurate classifier: is one that has an error rate of better than random guessing on new x values.
3) Two classifiers are diverse: if they make different errors on new data points

If the three classifiers are identical, i.e. not diverse, then when $h_1(x)$ is wrong $h_2(x)$ and $h_3(x)$ will also be wrong.

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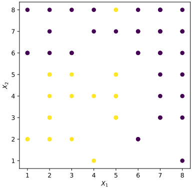
However, if the errors made by the classifiers are uncorrelated, then when $h_1(x)$ is wrong, $h_2(x)$ and $h_3(x)$ may be correct, so that a majority vote will correctly classify.

Error Probability of each model $= \varepsilon = 0.3$

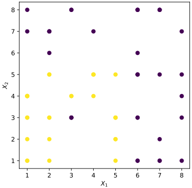
$$Pr(\text{ensemble being wrong}) = {}^3C_2(\varepsilon^2)(1-\varepsilon)^{3-2} + {}^3C_3(\varepsilon^3)(1-\varepsilon)^{3-3}$$

$$= 0.19 \leq 0.3$$

Round - 1



Round - 2



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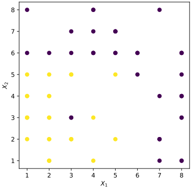

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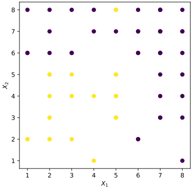

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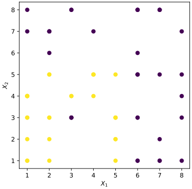

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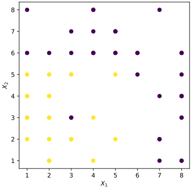

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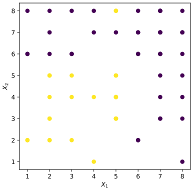

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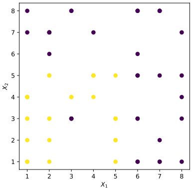

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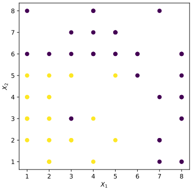

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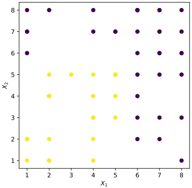

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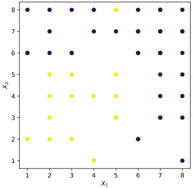

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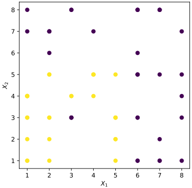

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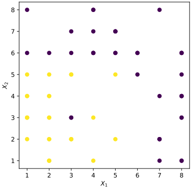

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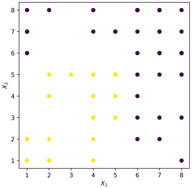

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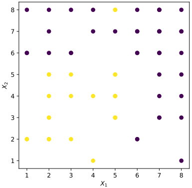

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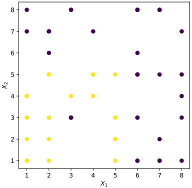

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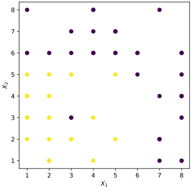

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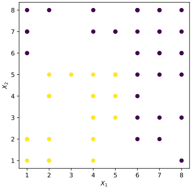

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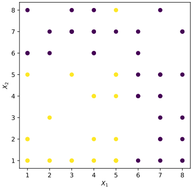

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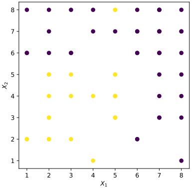

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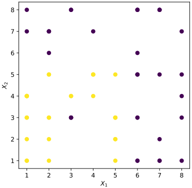
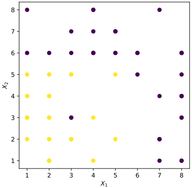


Round - 3



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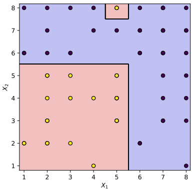
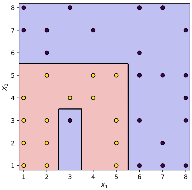


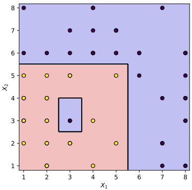
Tree Depth $= 4$

Round - 2



Tree Depth $= 5$

Round - 3



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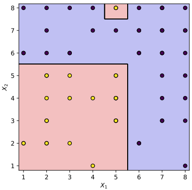

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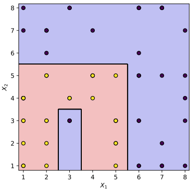
Round - 2



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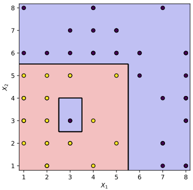

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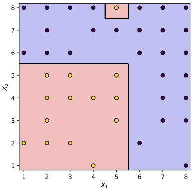

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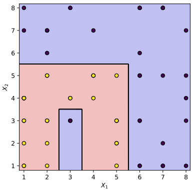

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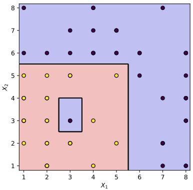
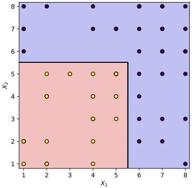


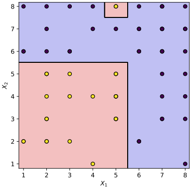
Tree Depth $= 5$

Round - 4



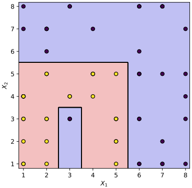
Tree Depth $= 2$

Round - 1



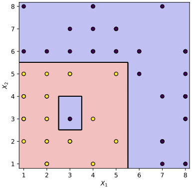
Tree Depth $= 4$

Round - 2



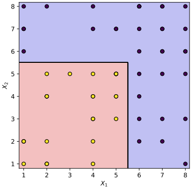
Tree Depth $= 5$

Round - 3



Tree Depth $= 5$

Round - 4



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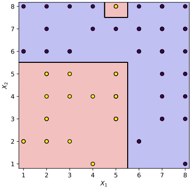
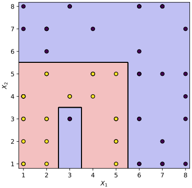


Tree Depth $= 4$

Round - 2



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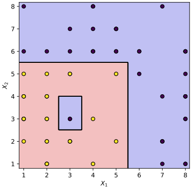

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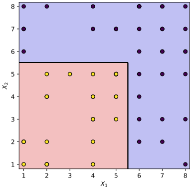
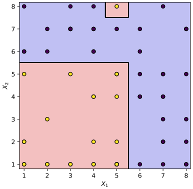
Round - 4



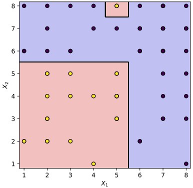
Tree Depth $= 2$

Round - 5



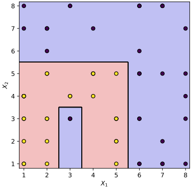
Tree Depth $= 4$

Round - 1



Tree Depth $= 4$

Round - 2



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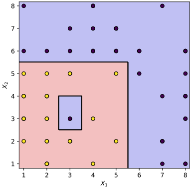
Round - 3



Tree Depth $= 5$

All learners are incrementally built.

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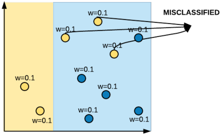
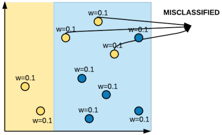
Incremental building: Incrementally try to classify “harder” samples correctly.



$$\alpha_1 = 0.42$$



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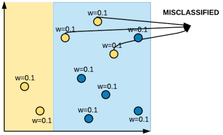

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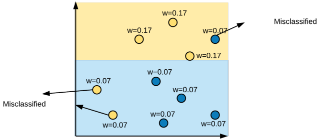
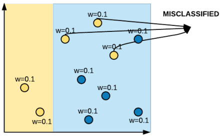


$$\alpha_2 = 0.66$$



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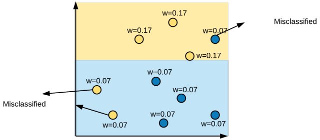

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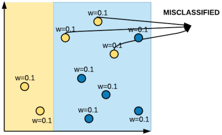

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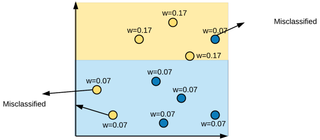

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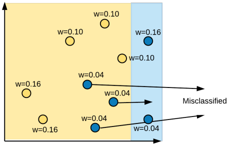
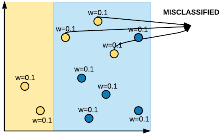


$$\alpha_3 = 0.99$$



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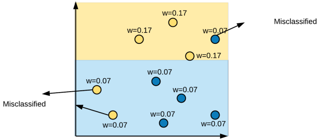

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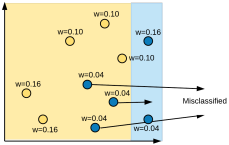

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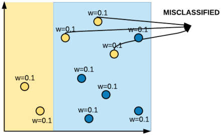

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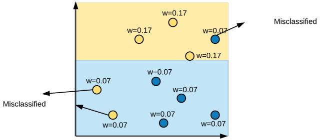

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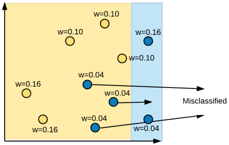

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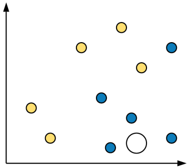

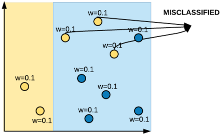

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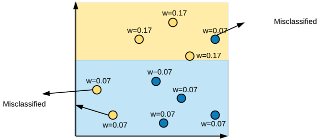

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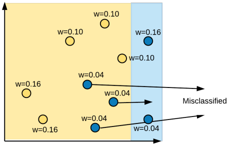
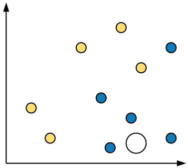
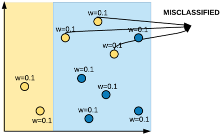


$$\alpha_3 = 0.99$$





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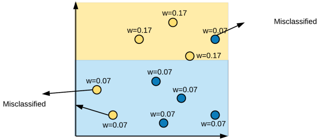

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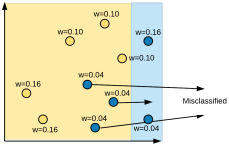

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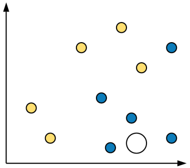

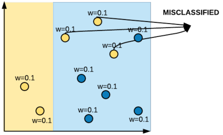

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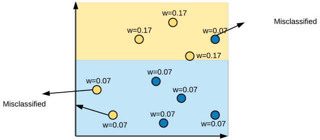

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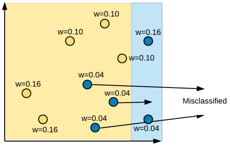
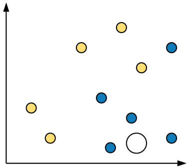
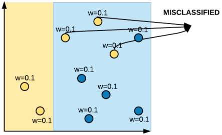


$$\alpha_3 = 0.99$$



Let us say, yellow class is $+1$ and blue class is -1



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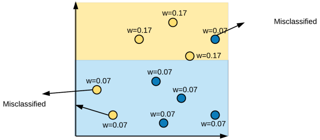

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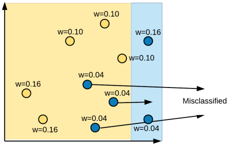

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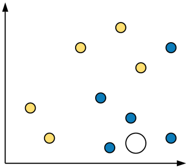
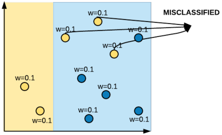


Let us say, yellow class is +1 and blue class is -1

Prediction = SIGN(0.42*-1 + 0.66*-1 + 0.99*+1) = Negative = blue



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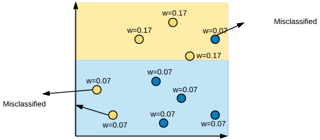

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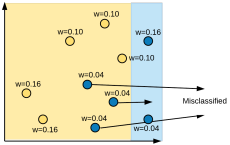
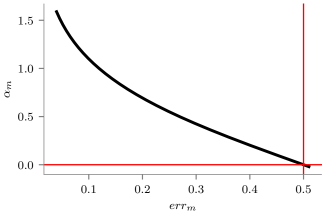
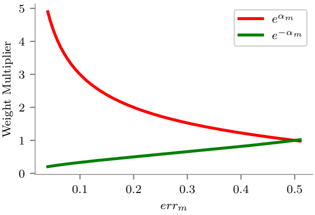


$$\alpha_3 = 0.99$$

Notebook: boosting-explanation.html



Notebook: boosting-explanation.html



ADABoost for regresion

From Paper: Improving Regressors using Boosting Techniques

Our problem will be that the modeling error is also nonzero because we have to determine the model in the presence of noise. Since we don't know the probability distributions, we approximate the expectation of the ME and PE using the sample ME (if the truth is known) and sample PE and then average over multiple experiments.

In the following discussion, we detail both bagging and boosting. We then discuss how to build trees which are the basic building blocks of our regression machines and use these ensembles on some standard test functions.

2. BAGGING

The following is a paraphrase of Breiman (1996b) with some difference in notation. Suppose we pick with replacement N_1 examples from the training set of size N_1 and call the k'th set of observations O_k. Based on these observations, we form a predictor $y^{(p)}(\mathbf{x},O_k)$. Because we are sampling with replacement, we may have multiple observations or no observations of a particular training example. Sampling with replacement is sometimes termed bootstrap sampling [Efron and Tibshirani (1993)] and therefore this method is called **b**ootstrap **agg**regating or bagging for short. The ensemble predictor is formed from the approximation to the expectation over all the observation sets, i.e. $E_O[y^{(p)}(\mathbf{x},O)]$ by using the average of the outputs of all the predictors. Breiman discusses which algorithms are good candidates for predictors and concludes that the best predictors are unstable, i.e., a small change in the training set O_k causes a large change in the predictor $y^{(p)}(\mathbf{x},O_k)$. Good candidates are regression trees and neural nets.

3. BOOSTING

In bagging, each training example is equally likely to be picked. In boosting, the probability of a particular example being in the training set of a particular machine depends on the performance of the prior machines on that example. The following is a modification of *Adaboost.R* [Freund and Schapire (1996a)].

Initially, to each training pattern we assign a weight $w_i=1 \quad i=1,\ldots,N_1$

Repeat the following while the average loss $\bar{L}$ defined

set. Each machine makes a hypothesis: $h_t:x\rightarrow y$

3. Pass *every* member of the training set through this machine to obtain a prediction $y_i^{(p)}(\mathbf{x}_i) \quad i=1,\ldots N_1$.

4. Calculate a loss for each training sample $L_i = L\left[\,|y_i^{(p)}(\mathbf{x}_i)-y_i|\,\right]$. The loss L may be of any functional form as long as $L\in[0,1]$. If we let

$$D = sup\,|y_i^{(p)}(\mathbf{x}_i) - y_i| \quad i=1,\ldots,N_1$$

then we have three candidate loss functions:

$$L_i = \frac{|y_i^{(p)}(\mathbf{x}_i) - y_i|}{D} \qquad (linear)$$

$$L_i = \frac{|y_i^{(p)}(\mathbf{x}_i) - y_i|^2}{D^2} \qquad (square\ \ law)$$

$$L_i = 1 - exp\left[\frac{-|y_i^{(p)}(\mathbf{x}_i) - y_i|}{D}\right] \qquad (exponential)$$

5. Calculate an average loss: $\bar{L} = \sum_{i=1}^{N_1} L_i p_i$

6. Form $\beta = \frac{\bar{L}}{1-\bar{L}}$. β is a measure of confidence in the predictor. Low β means high confidence in the prediction.

7. Update the weights: $w_i \rightarrow w_i\beta**[1-L_i]$, where ** indicates exponentiation. The smaller the loss, the more the weight is reduced making the probability smaller that this pattern will be picked as a member of the training set for the next machine in the ensemble.

8. For a particular input $\mathbf{x}_i$, each of the T machines makes a prediction h_t, $t=1,\ldots,T$. Obtain the cumulative prediction h_f using the T predictors:

Random Forest

- Random Forest is an ensemble of decision trees.

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- We have two types of bagging: bootstrap (on data) and random subspace (of features).

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- Random Forest is an ensemble of decision trees.
- We have two types of bagging: bootstrap (on data) and random subspace (of features).
- As features are randomly selected, we learn decorrelated trees and helps in reducing variance.

Random Forest

There are 3 parameters while training a random forest number of trees, number of features (m), maximum depth.

Training Algorithm

- For i^{th} tree ($i \in \{1 \cdots N\}$), select n samples from total N samples with replacement.

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- For i^{th} tree ($i \in \{1 \cdots N\}$), select n samples from total N samples with replacement.
- Learn Decision Tree on selected samples for i^{th} round.

Learning Decision Tree (for RF)

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There are 3 parameters while training a random forest number of trees, number of features (m), maximum depth.

Training Algorithm

- For i^{th} tree ($i \in \{1 \cdots N\}$), select n samples from total N samples with replacement.
- Learn Decision Tree on selected samples for i^{th} round.

Learning Decision Tree (for RF)

- For each split, select m features from total available M features and train a decision tree on selected features

Dataset

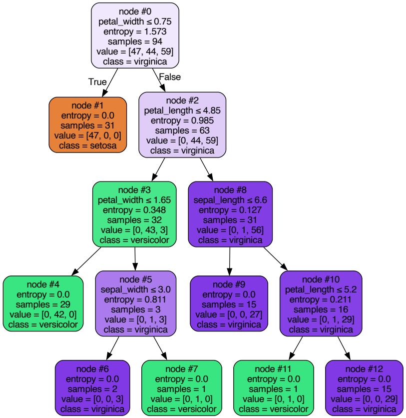
	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa
...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	virginica
146	6.3	2.5	5.0	1.9	virginica
147	6.5	3.0	5.2	2.0	virginica
148	6.2	3.4	5.4	2.3	virginica
149	5.9	3.0	5.1	1.8	virginica

150 rows × 5 columns

for *depth* in $[1, \ldots,$ *maximum depth* $]$

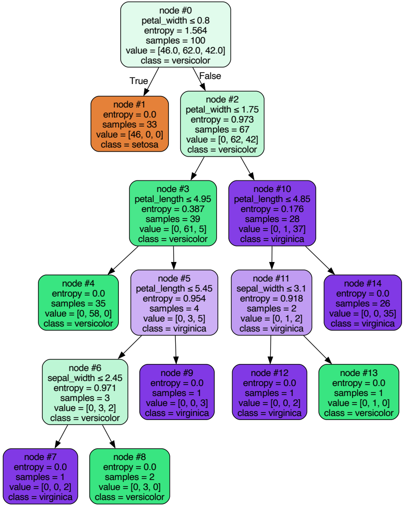
Decision Tree # 0

Notebook: ensemble-feature-importance.html



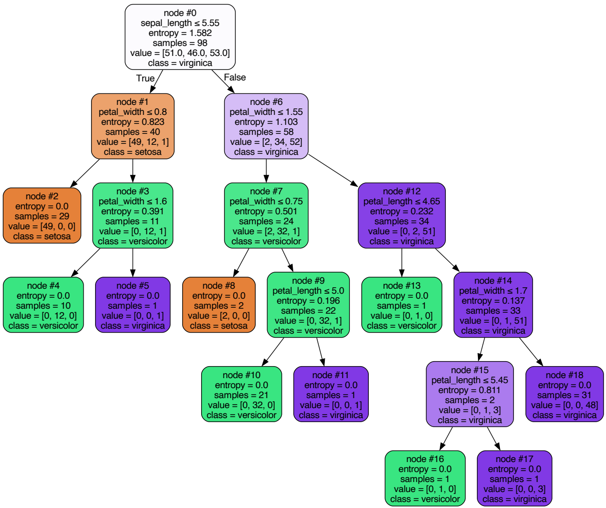
Decision Tree # 1

Notebook: ensemble-feature-importance.html



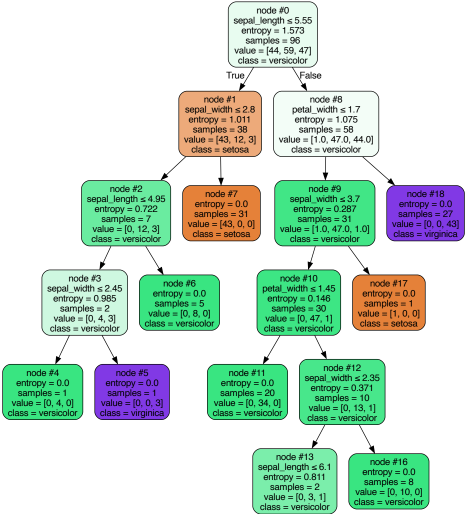
Decision Tree # 2

Notebook: ensemble-feature-importance.html



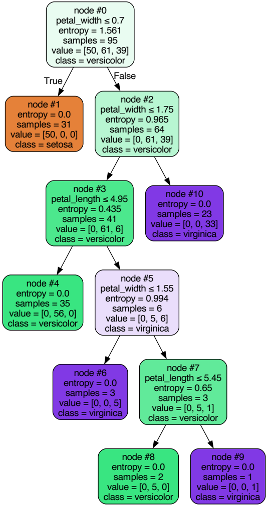
Decision Tree # 3

Notebook: ensemble-feature-importance.html



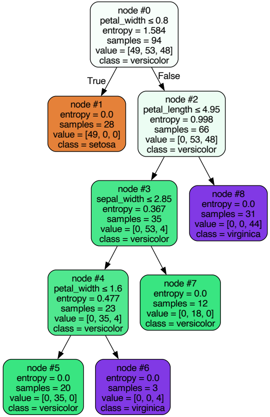
Decision Tree # 4

Notebook: ensemble-feature-importance.html



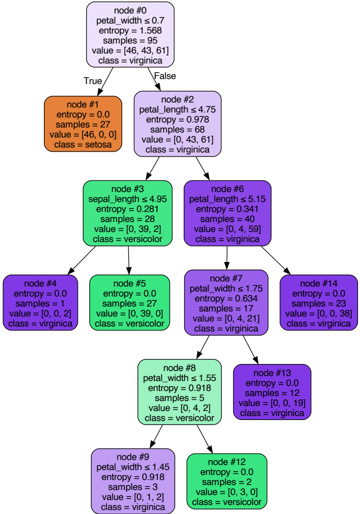
Decision Tree # 5

Notebook: ensemble-feature-importance.html



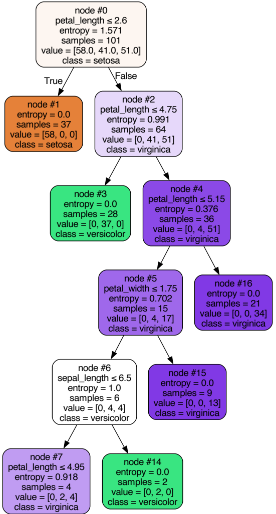
Decision Tree # 6

Notebook: ensemble-feature-importance.html



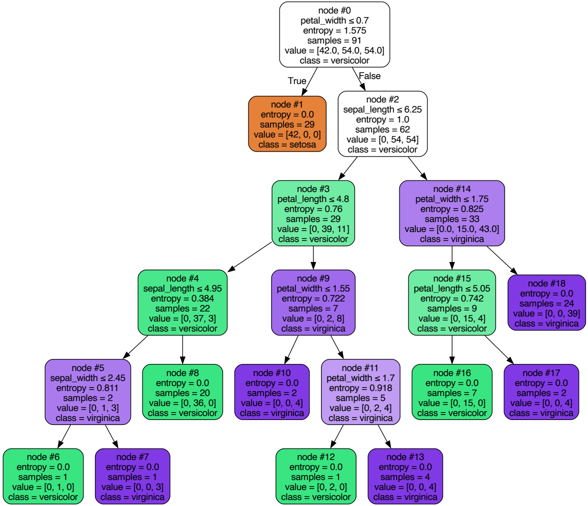
Decision Tree # 7

Notebook: ensemble-feature-importance.html



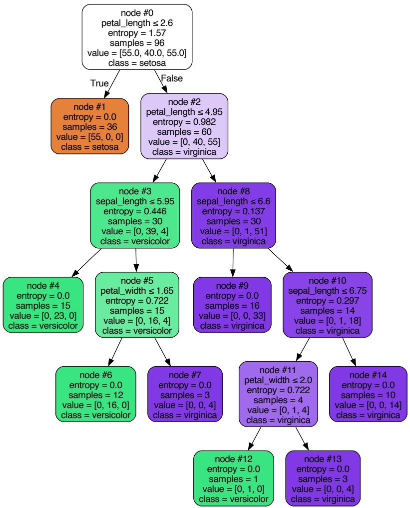
Decision Tree # 8

Notebook: ensemble-feature-importance.html

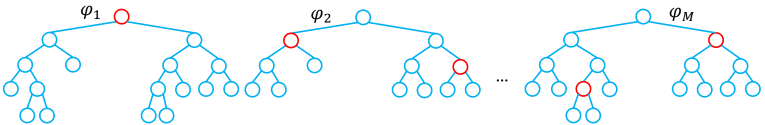


Decision Tree # 9

Notebook: ensemble-feature-importance.html



Feature Importance[1]



Importance of variable X_j for an ensemble of M trees φ_m is:

$$\text{Imp}(X_j) = \frac{1}{M} \sum_{m=1}^{M} \sum_{t \in \varphi_m} 1(j_t = j) \Big[p(t) \Delta i(t) \Big],$$

where j_t denotes the variable used at node t, $p(t) = N_t/N$ and $\Delta i(t)$ is the impurity reduction at node t:

$$\Delta i(t) = i(t) - \frac{N_{t_L}}{N_t} i(t_L) - \frac{N_{t_r}}{N_t} i(t_R)$$

[1] Slide Courtesy Gilles Louppe

Computed Feature Importance

Notebook: ensemble-feature-importance.html